

## Author Index to Volume 171

- Aguillon, F., V. Sidis and J.P. Gauyacq, Coupled-wavepacket study of model dissociative charge exchange in collisions between a diatomic ion and a diatomic molecule 171 (1993) 363
- Al Homsî-Teiar, S., see B. Pasquier 171 (1993) 203
- Amosov, K.A., S.A. Kochubei, K.N. Naumochkin, V.I. Makarov, I.V. Khmelinski and N.M. Bazhin, SO<sub>2</sub> fluorescence in cooled molecular beams under a magnetic field. The model analysis 171 (1993) 275
- Bazhin, N.M., see K.A. Amosov 171 (1993) 275
- Brion, C.E., see B.P. Hollebone 171 (1993) 303
- Buckingham, A.D., see S.A.C. McDowell 171 (1993) 89
- Čápek, V., Haken-Strobl-Reineker model: its limits of validity and a possible extension 171 (1993) 79
- Consalvo, D., J.W.I. van Bladel, R. Engeln and J. Reuss, Analysis of the torsional Raman spectrum of a pyramidal molecule, dimethylamine 171 (1993) 221
- Cosby, P.C., see M.J. Dyer 171 (1993) 237
- Davidson, E.R., see B.P. Hollebone 171 (1993) 303
- Decleva, P., see M. Ohno 171 (1993) 9
- Decleva, P., see A. Lisini 171 (1993) 159
- Defranceschi, M., see D. Mathieu 171 (1993) 133
- Delhalle, J., see D. Mathieu 171 (1993) 133
- Dick, B., Response functions and susceptibilities for multiresonant non-linear optical spectroscopy: perturbative computer algebra solution including feeding 171 (1993) 59
- Dietz, F., see N. Tyutyulkov 171 (1993) 293
- Dyer, M.J., G.W. Faris, P.C. Cosby, D.L. Huestis and T.G. Slanger, Optical excitation of the b <sup>4</sup>Σ<sup>-</sup>-X <sup>2</sup>Π transition in NO 171 (1993) 237
- Enders, A., see P. Pissis 171 (1993) 285
- Engeln, R., see D. Consalvo 171 (1993) 221
- Eriksson, L.A., see S. Lunell 171 (1993) 119
- Evseev, A.G., D.V. Kupriyanov, B.V. Picheyev, B.N. Sevastianov and O.S. Vasyutinskii, Orientation and alignment of metastable <sup>2</sup>P<sub>3/2</sub> thallium atoms following photodissociation of TlBr 171 (1993) 45
- Fängström, T., see S. Lunell 171 (1993) 119
- Faris, G.W., see M.J. Dyer 171 (1993) 237
- Feller, D., see B.P. Hollebone 171 (1993) 303
- Fillaux, F., see B. Pasquier 171 (1993) 203
- Fišer, J. and J. Vojtík, Ab initio CI calculation of nuclear quadrupole coupling constants of low-lying rovibrational levels in the X <sup>1</sup>Σ<sup>+</sup> state of CH<sup>+</sup> 171 (1993) 319

## Author Index to Volume 171

- Aguillon, F., V. Sidis and J.P. Gauyacq, Coupled-wavepacket study of model dissociative charge exchange in collisions between a diatomic ion and a diatomic molecule 171 (1993) 363
- Al Homsi-Teiar, S., see B. Pasquier 171 (1993) 203
- Amosov, K.A., S.A. Kochubei, K.N. Naumochkin, V.I. Makarov, I.V. Khmelinski and N.M. Bazhin, SO<sub>2</sub> fluorescence in cooled molecular beams under a magnetic field. The model analysis 171 (1993) 275
- Bazhin, N.M., see K.A. Amosov 171 (1993) 275
- Brion, C.E., see B.P. Hollebone 171 (1993) 303
- Buckingham, A.D., see S.A.C. McDowell 171 (1993) 89
- Čápek, V., Haken-Strobl-Reineker model: its limits of validity and a possible extension 171 (1993) 79
- Consalvo, D., J.W.I. van Bladel, R. Engeln and J. Reuss, Analysis of the torsional Raman spectrum of a pyramidal molecule, dimethylamine 171 (1993) 221
- Cosby, P.C., see M.J. Dyer 171 (1993) 237
- Davidson, E.R., see B.P. Hollebone 171 (1993) 303
- Decleva, P., see M. Ohno 171 (1993) 9
- Decleva, P., see A. Lisini 171 (1993) 159
- Defranceschi, M., see D. Mathieu 171 (1993) 133
- Delhalle, J., see D. Mathieu 171 (1993) 133
- Dick, B., Response functions and susceptibilities for multiresonant non-linear optical spectroscopy: perturbative computer algebra solution including feeding 171 (1993) 59
- Dietz, F., see N. Tyutyulkov 171 (1993) 293
- Dyer, M.J., G.W. Faris, P.C. Cosby, D.L. Huestis and T.G. Slanger, Optical excitation of the b <sup>4</sup>Σ<sup>-</sup>-X <sup>2</sup>Π transition in NO 171 (1993) 237
- Enders, A., see P. Pissis 171 (1993) 285
- Engeln, R., see D. Consalvo 171 (1993) 221
- Eriksson, L.A., see S. Lunell 171 (1993) 119
- Evseev, A.G., D.V. Kupriyanov, B.V. Picheyev, B.N. Sevastianov and O.S. Vasyutinskii, Orientation and alignment of metastable <sup>2</sup>P<sub>3/2</sub> thallium atoms following photodissociation of TlBr 171 (1993) 45
- Fängström, T., see S. Lunell 171 (1993) 119
- Faris, G.W., see M.J. Dyer 171 (1993) 237
- Feller, D., see B.P. Hollebone 171 (1993) 303
- Fillaux, F., see B. Pasquier 171 (1993) 203
- Fišer, J. and J. Vojtík, Ab initio CI calculation of nuclear quadrupole coupling constants of low-lying rovibrational levels in the X <sup>1</sup>Σ<sup>+</sup> state of CH<sup>+</sup> 171 (1993) 319

- Francisco, J.S. and G. Khitrov, An examination of the structure and inversion barrier for lithium and sodium phosphide 171 (1993) 153
- Fronzoni, G., see A. Lisini 171 (1993) 159
- Galasso, V., Ab initio calculations on the one- and two-photon electronic transitions of the conjugated isomers of benzene 171 (1993) 171
- Gallay, J., see N. Vekshin 171 (1993) 231
- Gatzweiler, W., see A. Pöppl 171 (1993) 375
- Gauyacq, J.P., see F. Aguillon 171 (1993) 363
- González-Luque, R., M. Merchán and B.O. Roos, A theoretical study of the collinear reaction  $F + H_2 \rightarrow HF + H$  using multiconfigurational second-order perturbation theory (CASPT2) 171 (1993) 107
- Grand, A., see D. Mathieu 171 (1993) 133
- Hermansson, K., see M.J. Wojcik 171 (1993) 189
- Hochstrasser, R.M., see K. Wynne 171 (1993) 179
- Hollebone, B.P., Y. Zheng, C.E. Brion, E.R. Davidson and D. Feller, Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using Hartree-Fock limit and configuration interaction wavefunctions for hydrogen fluoride 171 (1993) 303
- Holliday, K., see E. Vauthey 171 (1993) 253
- Huestis, D.L., see M.J. Dyer 171 (1993) 237
- Hüttermann, J., see A. Pöppl 171 (1993) 375
- Khitrov, G., see J.S. Francisco 171 (1993) 153
- Khmelinski, I.V., see K.A. Amosov 171 (1993) 275
- Klöpperpieper, A., see A. Pöppl 171 (1993) 375
- Kochubei, S.A., see K.A. Amosov 171 (1993) 275
- Krogh-Jespersen, K., see M.J. Smith 171 (1993) 97
- Kupriyanov, D.V. and O.S. Vasyutinskii, Orientation and alignment of  $^2P_{3/2}$  fragments following photodissociation of heteroatomic molecules 171 (1993) 25
- Kupriyanov, D.V., see A.G. Evseev 171 (1993) 45
- Le Calvé, N., see B. Pasquier 171 (1993) 203
- Lecayon, G., see D. Mathieu 171 (1993) 133
- Levy, R.M., see M.J. Smith 171 (1993) 97
- Liang, C., see M. Shen 171 (1993) 325
- Lindgren, J., see M.J. Wojcik 171 (1993) 189
- Lisini, A., P. Decleva and G. Fronzoni, Quasidegenerate perturbation theory applied to the calculation of excitation spectra 171 (1993) 159
- Lund, A., see S. Lunell 171 (1993) 119
- Lunell, S., L.A. Eriksson, T. Fängström, J. Maruani, L. Sjöqvist and A. Lund, Theoretical investigation of the structure and dynamics of the cyclopentane radical cation 171 (1993) 119
- Makarov, V.I., see K.A. Amosov 171 (1993) 275
- Maruani, J., see S. Lunell 171 (1993) 119

- Mathieu, D., M. Defranceschi, G. Lecayon, A. Grand and J. Delhalle, Dependence of the vibrational frequencies and intensities on the configuration of polyacrylonitrile: an ab initio study on model oligomers 171 (1993) 133
- McDowell, S.A.C. and A.D. Buckingham, Isotope effects on the stability of the nitrogen-acetylene van der Waals dimer 171 (1993) 89
- Merchán, M., see R. González-Luque 171 (1993) 107
- Naumochkin, K.N., see K.A. Amosov 171 (1993) 275
- Nimtz, G., see P. Pissis 171 (1993) 285
- Offer, A.R., see J. Schleipen 171 (1993) 347
- Ohno, M. and P. Decleva, Cooperative core hole screening mechanism in adsorbates: its hindrance in the NEXAFS spectra of the CO/Ni and N<sub>2</sub>/Ni systems 171 (1993) 9
- Ojamäe, L., see M.J. Wojcik 171 (1993) 189
- Pasquier, B., N. Le Calvé, S. Al Homsî-Teïar and F. Fillaux, Vibrational study of various crystalline phases of thallium dihydrogen phosphate TiH<sub>2</sub>PO<sub>4</sub> and its deuterated analog TiD<sub>2</sub>PO<sub>4</sub> 171 (1993) 203
- Petelenz, P., Electro-absorption spectra of degenerate charge transfer states 171 (1993) 397
- Picheyev, B.V., see A.G. Evseev 171 (1993) 45
- Pissis, P., A. Enders and G. Nimtz, Hydration dependence of molecular mobility in phospholipid bilayers 171 (1993) 285
- Pöpl, A., G. Völkel, O. Tober, A. Klöpperpieper, J. Hüttermann and W. Gatzweiler, <sup>1</sup>H and <sup>2</sup>D electron nuclear double resonance (ENDOR) and electron spin echo envelope modulation (ESEEM) investigations on γ-irradiated betaine arsenate 171 (1993) 375
- Pöpl, A. and G. Völkel, <sup>14</sup>N ENDOR study of γ-irradiated betaine arsenate 171 (1993) 387
- Power, E.A. and T. Thirunamachandran, A new insight into the mechanism of intermolecular forces 171 (1993) 1
- Renn, A., see E. Vauthey 171 (1993) 253
- Reuss, J., see D. Consalvo 171 (1993) 221
- Roos, B.O., see R. González-Luque 171 (1993) 107
- Schaefer III, H.F., see M. Shen 171 (1993) 325
- Schleipen, J., J.J. ter Meulen and A.R. Offer, State-to-state cross sections for rotational excitation of ortho- and para-NH<sub>3</sub> by ortho- and para-H<sub>2</sub>. Experiment versus theory 171 (1993) 347
- Sevastianov, B.N., see A.G. Evseev 171 (1993) 45
- Shalabi, A.S. and M.M. Shalabi, Calculations on clusters of Li and F ions at LiF crystal geometries 171 (1993) 145
- Shalabi, M.M., see A.S. Shalabi 171 (1993) 145
- Shen, M., C. Liang and H.F. Schaefer III, The tetramer of borane and its heavier valence-isoelectronic analogs: M<sub>4</sub>H<sub>12</sub> with M=B, Al, and Ga 171 (1993) 325
- Sidis, V., see F. Aguillon 171 (1993) 363
- Sjöqvist, L., see S. Lunell 171 (1993) 119
- Slinger, T.G., see M.J. Dyer 171 (1993) 237
- Smith, M.J., K. Krogh-Jespersen and R.M. Levy, Solvent effects on the torsional dynamics of a twisted intramolecular charge transfer (TICT) molecule: bianthryl in acetonitrile 171 (1993) 97

- Ter Meulen, J.J., see J. Schleipen 171 (1993) 347
- Thirunamachandran, T., see E.A. Power 171 (1993) 1
- Tober, O., see A. Pöpl 171 (1993) 375
- Tyutyulkov, N. and F. Dietz, Energy gap equation of 1D polyconjugated  $\pi$ -systems in the Hubbard approximation 171 (1993) 293
- Van Bladel, J.W.I., see D. Consalvo 171 (1993) 221
- Vasyutinskii, O.S., see D.V. Kupriyanov 171 (1993) 25
- Vasyutinskii, O.S., see A.G. Evseev 171 (1993) 45
- Vauthey, E., K. Holliday, C. Wei, A. Renn and U.P. Wild, Stark effect and spectral hole-burning: solvation of organic dyes in polymers 171 (1993) 253
- Vekshin, N., M. Vincent and J. Gallay, Tyrosine hypochromism and absence of tyrosine-tryptophan energy transfer in phospholipase A<sub>2</sub> and ribonuclease T<sub>1</sub> 171 (1993) 231
- Vincent, M., see N. Vekshin 171 (1993) 231
- Vojtik, J., see J. Fišer 171 (1993) 319
- Völkel, G., see A. Pöpl 171 (1993) 375
- Völkel, G., see A. Pöpl 171 (1993) 387
- Wei, C., see E. Vauthey 171 (1993) 253
- Wild, U.P., see E. Vauthey 171 (1993) 253
- Wojcik, M.J., K. Hermansson, J. Lindgren and L. Ojamäe, Theoretical simulation of OH and OD stretching bands of isotopically diluted HDO molecules in aqueous solution 171 (1993) 189
- Wynne, K. and R.M. Hochstrasser, Coherence effects in the anisotropy of optical experiments 171 (1993) 179
- Zabarnick, S., Kinetics of the reaction  $\text{OH} + \text{NO} + \text{M} \rightarrow \text{HONO} + \text{M}$  as a function of temperature and pressure in the presence of argon, SF<sub>6</sub>, and N<sub>2</sub> bath gas 171 (1993) 265
- Zheng, Y., see B.P. Hollebhone 171 (1993) 303

## Subject Index to Volume 171

### Methods

#### Theoretical

##### *Quantized field theory*

- A new insight into the mechanism of intermolecular forces, E.A. Power and T. Thirunamachandran 171 (1993) 1

##### *Many body and quasiparticle approaches*

- Cooperative core hole screening mechanism in adsorbates: its hindrance in the NEXAFS spectra of the CO/Ni and N<sub>2</sub>/Ni systems, M. Ohno and P. Decleva 171 (1993) 9
- Energy gap equation of 1D polyconjugated  $\pi$ -systems in the Hubbard approximation, N. Tyutyulkov and F. Dietz 171 (1993) 293
- Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using Hartree-Fock limit and configuration interaction wavefunctions for hydrogen fluoride, B.P. Hollebone, Y. Zheng, C.E. Brion, E.R. Davidson and D. Feller 171 (1993) 303

##### *Coupling schemes and perturbative treatments*

- Orientation and alignment of  $^2P_{3/2}$  fragments following photodissociation of heteroatomic molecules, D.V. Kupriyanov and O.S. Vasyutinskii 171 (1993) 25
- Orientation and alignment of metastable  $^2P_{3/2}$  thallium atoms following photodissociation of TlBr, A.G. Evseev, D.V. Kupriyanov, B.V. Picheyev, B.N. Sevastianov and O.S. Vasyutinskii 171 (1993) 45
- Response functions and susceptibilities for multiresonant non-linear optical spectroscopy: perturbative computer algebra solution including feeding, B. Dick 171 (1993) 59

##### *Transport quantum mechanics*

- Haken-Strobl-Reineker model: its limits of validity and a possible extension, V. Čápek 171 (1993) 79

##### *Ab initio schemes for stationary properties*

- Isotope effects on the stability of the nitrogen-acetylene van der Waals dimer, S.A.C. McDowell and A.D. Buckingham 171 (1993) 89
- Solvent effects on the torsional dynamics of a twisted intramolecular charge transfer (TICT) molecule: bianthryl in acetonitrile, M.J. Smith, K. Krogh-Jespersen and R.M. Levy 171 (1993) 97
- A theoretical study of the collinear reaction  $F + H_2 \rightarrow HF + H$  using multiconfigurational second-order perturbation theory (CASPT2), R. González-Luque, M. Merchán and B.O. Roos 171 (1993) 107
- Theoretical investigation of the structure and dynamics of the cyclopentane radical cation, S. Lunell, L.A. Eriksson, T. Fängström, J. Maruani, L. Sjöqvist and A. Lund 171 (1993) 119

- Dependence of the vibrational frequencies and intensities on the configuration of polyacrylonitrile: an ab initio study on model oligomers, D. Mathieu, M. Defranceschi, G. Lecayon, A. Grand and J. Delhalle 171 (1993) 133
- Calculations on clusters of Li and F ions at LiF crystal geometries, A.S. Shalabi and M.M. Shalabi 171 (1993) 145
- An examination of the structure and inversion barrier for lithium and sodium phosphide, J.S. Francisco and G. Khitrov 171 (1993) 153
- Quasidegenerate perturbation theory applied to the calculation of excitation spectra, A. Lisini, P. Decleva and G. Fronzoni 171 (1993) 159
- Ab initio calculations on the one- and two-photon electronic transitions of the conjugated isomers of benzene, V. Galasso 171 (1993) 171
- Ab initio CI calculation of nuclear quadrupole coupling constants of low-lying rovibrational levels in the X  $^1\Sigma^+$  state of  $\text{CH}^+$ , J. Fišer and J. Vojtík 171 (1993) 319
- The tetramer of borane and its heavier valence-isoelectronic analogs:  $\text{M}_4\text{H}_{12}$  with  $\text{M}=\text{B}$ , Al, and Ga, M. Shen, C. Liang and H.F. Schaefer III 171 (1993) 325

#### *Computational and simulation methods*

- Isotope effects on the stability of the nitrogen-acetylene van der Waals dimer, S.A.C. McDowell and A.D. Buckingham 171 (1993) 89
- Solvent effects on the torsional dynamics of a twisted intramolecular charge transfer (TICT) molecule: bianthryl in acetonitrile, M.J. Smith, K. Krogh-Jespersen and R.M. Levy 171 (1993) 97
- A theoretical study of the collinear reaction  $\text{F} + \text{H}_2 \rightarrow \text{HF} + \text{H}$  using multiconfigurational second-order perturbation theory (CASPT2), R. González-Luque, M. Merchán and B.O. Roos 171 (1993) 107
- Coherence effects in the anisotropy of optical experiments, K. Wynne and R.M. Hochstrasser 171 (1993) 179
- Theoretical simulation of OH and OD stretching bands of isotopically diluted HDO molecules in aqueous solution, M.J. Wojcik, K. Hermansson, J. Lindgren and L. Ojamäe 171 (1993) 189
- Energy gap equation of 1D polyconjugated  $\pi$ -systems in the Hubbard approximation, N. Tyutyulkov and F. Dietz 171 (1993) 293
- Ab initio CI calculation of nuclear quadrupole coupling constants of low-lying rovibrational levels in the X  $^1\Sigma^+$  state of  $\text{CH}^+$ , J. Fišer and J. Vojtík 171 (1993) 319
- The tetramer of borane and its heavier valence-isoelectronic analogs:  $\text{M}_4\text{H}_{12}$  with  $\text{M}=\text{B}$ , Al, and Ga, M. Shen, C. Liang and H.F. Schaefer III 171 (1993) 325

#### *Molecular dynamics and scattering theory*

- Orientation and alignment of  $^2\text{P}_{3/2}$  fragments following photodissociation of heteroatomic molecules, D.V. Kupriyanov and O.S. Vasyutinskii 171 (1993) 25
- State-to-state cross sections for rotational excitation of ortho- and para- $\text{NH}_3$  by ortho- and para- $\text{H}_2$ . Experiment versus theory, J. Schleipen, J.J. ter Meulen and A.R. Offer 171 (1993) 347
- Coupled-wavepacket study of model dissociative charge exchange in collisions between a diatomic ion and a diatomic molecule, F. Aguillon, V. Sidis and J.P. Gauyacq 171 (1993) 363

#### **Experimental**

##### *Magnetic resonances*

- Theoretical investigation of the structure and dynamics of the cyclopentane radical cation, S. Lunell, L.A. Eriksson, T. Fängström, J. Maruani, L. Sjöqvist and A. Lund 171 (1993) 119



- <sup>1</sup>H and <sup>2</sup>D electron nuclear double resonance (ENDOR) and electron spin echo envelope modulation (ESEEM) investigations on  $\gamma$ -irradiated betaine arsenate, A. Pöpl, G. Völkel, O. Tober, A. Klöpperpieper, J. Hüttermann and W. Gatzweiler 171 (1993) 375
- <sup>14</sup>N ENDOR study of  $\gamma$ -irradiated betaine arsenate, A. Pöpl and G. Völkel 171 (1993) 387
- Infrared spectroscopy*
- Dependence of the vibrational frequencies and intensities on the configuration of polyacrylonitrile: an ab initio study on model oligomers, D. Mathieu, M. Defranceschi, G. Lecayon, A. Grand and J. Delhalle 171 (1993) 133
- Vibrational study of various crystalline phases of thallium dihydrogen phosphate  $\text{TiH}_2\text{PO}_4$  and its deuterated analog  $\text{TID}_2\text{PO}_4$ , B. Pasquier, N. Le Calvé, S. Al Homsî-Teïar and F. Fillaux 171 (1993) 203
- Raman spectroscopy*
- Vibrational study of various crystalline phases of thallium dihydrogen phosphate  $\text{TiH}_2\text{PO}_4$  and its deuterated analog  $\text{TID}_2\text{PO}_4$ , B. Pasquier, N. Le Calvé, S. Al Homsî-Teïar and F. Fillaux 171 (1993) 203
- Analysis of the torsional Raman spectrum of a pyramidal molecule, dimethylamine, D. Consalvo, J.W.I. van Bladel, R. Engeln and J. Reuss 171 (1993) 221
- Visible and UV spectroscopy*
- Tyrosine hypochromism and absence of tyrosine-tryptophan energy transfer in phospholipase  $\text{A}_2$  and ribonuclease  $\text{T}_1$ , N. Vekshin, M. Vincent and J. Gallay 171 (1993) 231
- Optical excitation of the  $\text{b } ^4\Sigma^- - \text{X } ^2\Pi$  transition in NO, M.J. Dyer, G.W. Faris, P.C. Cosby, D.L. Huestis and T.G. Slanger 171 (1993) 237
- Stark effect and spectral hole-burning: solvation of organic dyes in polymers, E. Vauthey, K. Holliday, C. Wei, A. Renn and U.P. Wild 171 (1993) 253
- Electro-absorption spectra of degenerate charge transfer states, P. Petelenz 171 (1993) 397
- Fluorescence spectroscopy*
- Tyrosine hypochromism and absence of tyrosine-tryptophan energy transfer in phospholipase  $\text{A}_2$  and ribonuclease  $\text{T}_1$ , N. Vekshin, M. Vincent and J. Gallay 171 (1993) 231
- Kinetics of the reaction  $\text{OH} + \text{NO} + \text{M} \rightarrow \text{HONO} + \text{M}$  as a function of temperature and pressure in the presence of argon,  $\text{SF}_6$ , and  $\text{N}_2$  bath gas, S. Zabarnick 171 (1993) 265
- $\text{SO}_2$  fluorescence in cooled molecular beams under a magnetic field. The model analysis, K.A. Amosov, S.A. Kochubei, K.N. Naumochkin, V.I. Makarov, I.V. Khmelinski and N.M. Bazhin 171 (1993) 275
- Electron impact spectroscopy*
- Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using Hartree-Fock limit and configuration interaction wavefunctions for hydrogen fluoride, B.P. Hollebone, Y. Zheng, C.E. Brion, E.R. Davidson and D. Feller 171 (1993) 303
- Laser methods*
- Kinetics of the reaction  $\text{OH} + \text{NO} + \text{M} \rightarrow \text{HONO} + \text{M}$  as a function of temperature and pressure in the presence of argon,  $\text{SF}_6$ , and  $\text{N}_2$  bath gas, S. Zabarnick 171 (1993) 265



*Coherent optical spectroscopy*

- Coherence effects in the anisotropy of optical experiments, K. Wynne and R.M. Hochstrasser 171 (1993) 179

*Optical pumping*

- Orientation and alignment of metastable  $^2P_{3/2}$  thallium atoms following photodissociation of TlBr, A.G. Evseev, D.V. Kupriyanov, B.V. Picheyev, B.N. Sevastianov and O.S. Vasyutinskii 171 (1993) 45
- Optical excitation of the  $b\ ^4\Sigma^- - X\ ^2\Pi$  transition in NO, M.J. Dyer, G.W. Faris, P.C. Cosby, D.L. Huestis and T.G. Slanger 171 (1993) 237

*Atomic and molecular beam techniques*

- State-to-state cross sections for rotational excitation of ortho- and para-NH<sub>3</sub> by ortho- and para-H<sub>2</sub>. Experiment versus theory, J. Schleipen, J.J. ter Meulen and A.R. Offer 171 (1993) 347

*Time-resolved experiments*

- Orientation and alignment of metastable  $^2P_{3/2}$  thallium atoms following photodissociation of TlBr, A.G. Evseev, D.V. Kupriyanov, B.V. Picheyev, B.N. Sevastianov and O.S. Vasyutinskii 171 (1993) 45
- Coherence effects in the anisotropy of optical experiments, K. Wynne and R.M. Hochstrasser 171 (1993) 179
- Kinetics of the reaction  $OH + NO + M \rightarrow HONO + M$  as a function of temperature and pressure in the presence of argon, SF<sub>6</sub>, and N<sub>2</sub> bath gas, S. Zabarnick 171 (1993) 265
- Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using Hartree-Fock limit and configuration interaction wavefunctions for hydrogen fluoride, B.P. Hollebone, Y. Zheng, C.E. Brion, E.R. Davidson and D. Feller 171 (1993) 303

*Measurement of macroscopic variables*

- Hydration dependence of molecular mobility in phospholipid bilayers, P. Pissis, A. Enders and G. Nimtz 171 (1993) 285

**Objects****Bulk systems***Gases*

- Analysis of the torsional Raman spectrum of a pyramidal molecule, dimethylamine, D. Consalvo, J.W.I. van Bladel, R. Engeln and J. Reuss 171 (1993) 221

*Supersonic beams*

- Isotope effects on the stability of the nitrogen-acetylene van der Waals dimer, S.A.C. McDowell and A.D. Buckingham 171 (1993) 89
- SO<sub>2</sub> fluorescence in cooled molecular beams under a magnetic field. The model analysis, K.A. Amosov, S.A. Kochubei, K.N. Naumochkin, V.I. Makarov, I.V. Khmelinski and N.M. Bazhin 171 (1993) 275

*Liquids mixtures and solutions*

- Solvent effects on the torsional dynamics of a twisted intramolecular charge transfer (TICT) molecule: bianthryl in acetonitrile, M.J. Smith, K. Krogh-Jespersen and R.M. Levy 171 (1993) 97
- Theoretical simulation of OH and OD stretching bands of isotopically diluted HDO molecules in aqueous solution, M.J. Wojcik, K. Hermansson, J. Lindgren and L. Ojamäe 171 (1993) 189

*Crystals*

- Calculations on clusters of Li and F ions at LiF crystal geometries, A.S. Shalabi and M.M. Shalabi 171 (1993) 145
- Vibrational study of various crystalline phases of thallium dihydrogen phosphate  $\text{TiH}_2\text{PO}_4$  and its deuterated analog  $\text{TlD}_2\text{PO}_4$ , B. Pasquier, N. Le Calvé, S. Al Homsî-Teïar and F. Fillaux 171 (1993) 203

*-neat*

- Electro-absorption spectra of degenerate charge transfer states, P. Petelenz 171 (1993) 397

*Glasses*

- Stark effect and spectral hole-burning: solvation of organic dyes in polymers, E. Vauthey, K. Holliday, C. Wei, A. Renn and U.P. Wild 171 (1993) 253

*Liquid crystals*

- Hydration dependence of molecular mobility in phospholipid bilayers, P. Pissis, A. Enders and G. Nimtz 171 (1993) 285

*Polymers*

- Dependence of the vibrational frequencies and intensities on the configuration of polyacrylonitrile: an ab initio study on model oligomers, D. Mathieu, M. Defranceschi, G. Lecayon, A. Grand and J. Delhalle 171 (1993) 133
- Stark effect and spectral hole-burning: solvation of organic dyes in polymers, E. Vauthey, K. Holliday, C. Wei, A. Renn and U.P. Wild 171 (1993) 253
- Energy gap equation of 1D polyconjugated  $\pi$ -systems in the Hubbard approximation, N. Tyutyulkov and F. Dietz 171 (1993) 293

*Semiconductors*

- An examination of the structure and inversion barrier for lithium and sodium phosphide, J.S. Francisco and G. Khitrov 171 (1993) 153

*Surfaces*

- Calculations on clusters of Li and F ions at LiF crystal geometries, A.S. Shalabi and M.M. Shalabi 171 (1993) 145

*Dielectrics*

- $^1\text{H}$  and  $^2\text{D}$  electron nuclear double resonance (ENDOR) and electron spin echo envelope modulation (ESEEM) investigations on  $\gamma$ -irradiated betaine arsenate, A. Pöpl, G. Völkel, O. Tober, A. Klöpperpieper, J. Hüttermann and W. Gatzweiler 171 (1993) 375
- $^{14}\text{N}$  ENDOR study of  $\gamma$ -irradiated betaine arsenate, A. Pöpl and G. Völkel 171 (1993) 387

*Biological systems*

- Haken–Strobl–Reineker model: its limits of validity and a possible extension, V. Čápek 171 (1993) 79  
 Tyrosine hypochromism and absence of tyrosine–tryptophan energy transfer in phospholipase A<sub>2</sub> and ribonuclease T<sub>1</sub>, N. Vekshin, M. Vincent and J. Gallay 171 (1993) 231  
 Hydration dependence of molecular mobility in phospholipid bilayers, P. Pissis, A. Enders and G. Nimtz 171 (1993) 285

*Microscopic systems**Atoms*

- Quasidegenerate perturbation theory applied to the calculation of excitation spectra, A. Lisini, P. Decleva and G. Fronzoni 171 (1993) 159

*Molecules (neutral and ionic)*

- Haken–Strobl–Reineker model: its limits of validity and a possible extension, V. Čápek 171 (1993) 79  
 Quasidegenerate perturbation theory applied to the calculation of excitation spectra, A. Lisini, P. Decleva and G. Fronzoni 171 (1993) 159  
 Stark effect and spectral hole-burning: solvation of organic dyes in polymers, E. Vauthey, K. Holliday, C. Wei, A. Renn and U.P. Wild 171 (1993) 253  
 Ab initio CI calculation of nuclear quadrupole coupling constants of low-lying rovibrational levels in the X <sup>1</sup>Σ<sup>+</sup> state of CH<sup>+</sup>, J. Fišer and J. Vojtík 171 (1993) 319

*–diatomic*

- Orientation and alignment of <sup>2</sup>P<sub>3/2</sub> fragments following photodissociation of heteroatomic molecules, D.V. Kupriyanov and O.S. Vasyutinskii 171 (1993) 25  
 Orientation and alignment of metastable <sup>2</sup>P<sub>3/2</sub> thallium atoms following photodissociation of TlBr, A.G. Evseev, D.V. Kupriyanov, B.V. Picheyev, B.N. Sevastianov and O.S. Vasyutinskii 171 (1993) 45  
 Optical excitation of the b <sup>4</sup>Σ<sup>−</sup>–X <sup>2</sup>Π transition in NO, M.J. Dyer, G.W. Faris, P.C. Cosby, D.L. Huestis and T.G. Slanger 171 (1993) 237  
 Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using Hartree–Fock limit and configuration interaction wavefunctions for hydrogen fluoride, B.P. Hollebone, Y. Zheng, C.E. Brion, E.R. Davidson and D. Feller 171 (1993) 303  
 Coupled-wavepacket study of model dissociative charge exchange in collisions between a diatomic ion and a diatomic molecule, F. Aguillon, V. Sidis and J.P. Gauyacq 171 (1993) 363

*–small polyatomics*

- A theoretical study of the collinear reaction F + H<sub>2</sub> → HF + H using multiconfigurational second-order perturbation theory (CASPT2), R. González-Luque, M. Merchán and B.O. Roos 171 (1993) 107  
 An examination of the structure and inversion barrier for lithium and sodium phosphide, J.S. Francisco and G. Khitrov 171 (1993) 153  
 Ab initio calculations on the one- and two-photon electronic transitions of the conjugated isomers of benzene, V. Galasso 171 (1993) 171  
 Analysis of the torsional Raman spectrum of a pyramidal molecule, dimethylamine, D. Consalvo, J.W.I. van Bladel, R. Engeln and J. Reuss 171 (1993) 221

- SO<sub>2</sub> fluorescence in cooled molecular beams under a magnetic field. The model analysis, K.A. Amosov, S.A. Kochubei, K.N. Naumochkin, V.I. Makarov, I.V. Khmelinski and N.M. Bazhin 171 (1993) 275
- The tetramer of borane and its heavier valence-isoelectronic analogs: M<sub>4</sub>H<sub>12</sub> with M=B, Al, and Ga, M. Shen, C. Liang and H.F. Schaefer III 171 (1993) 325
- polymeric and biological*
- Tyrosine hypochromism and absence of tyrosine-tryptophan energy transfer in phospholipase A<sub>2</sub> and ribonuclease T<sub>1</sub>, N. Vekshin, M. Vincent and J. Gallay 171 (1993) 231
- Energy gap equation of 1D polyconjugated  $\pi$ -systems in the Hubbard approximation, N. Tyutyulkov and F. Dietz 171 (1993) 293
- Molecular aggregates*
- Haken-Strobl-Reineker model: its limits of validity and a possible extension, V. Čápek 171 (1993) 79
- dimers*
- Electro-absorption spectra of degenerate charge transfer states, P. Petelenz 171 (1993) 397
- van der Waals molecules*
- Isotope effects on the stability of the nitrogen-acetylene van der Waals dimer, S.A.C. McDowell and A.D. Buckingham 171 (1993) 89
- clusters*
- Cooperative core hole screening mechanism in adsorbates: its hindrance in the NEXAFS spectra of the CO/Ni and N<sub>2</sub>/Ni systems, M. Ohno and P. Decleva 171 (1993) 9
- Calculations on clusters of Li and F ions at LiF crystal geometries, A.S. Shalabi and M.M. Shalabi 171 (1993) 145
- complexes*
- An examination of the structure and inversion barrier for lithium and sodium phosphide, J.S. Francisco and G. Khitrov 171 (1993) 153
- Free radicals (including hydronium and muonium)*
- Theoretical investigation of the structure and dynamics of the cyclopentane radical cation, S. Lunell, L.A. Eriksson, T. Fängström, J. Maruani, L. Sjöqvist and A. Lund 171 (1993) 119
- Kinetics of the reaction OH+NO+M→HONO+M as a function of temperature and pressure in the presence of argon, SF<sub>6</sub>, and N<sub>2</sub> bath gas, S. Zabarnick 171 (1993) 265
- <sup>1</sup>H and <sup>2</sup>D electron nuclear double resonance (ENDOR) and electron spin echo envelope modulation (ESEEM) investigations on  $\gamma$ -irradiated betaine arsenate, A. Pöpl, G. Völkel, O. Tober, A. Klöpperpieper, J. Hüttermann and W. Gatzweiler 171 (1993) 375
- <sup>14</sup>N ENDOR study of  $\gamma$ -irradiated betaine arsenate, A. Pöpl and G. Völkel 171 (1993) 387
- Quasiparticles (including excitations)*
- Electro-absorption spectra of degenerate charge transfer states, P. Petelenz 171 (1993) 397
- Defects and impurities*
- Calculations on clusters of Li and F ions at LiF crystal geometries, A.S. Shalabi and M.M. Shalabi 171 (1993) 145

## Phenomena

### *Molecular structure*

- Theoretical investigation of the structure and dynamics of the cyclopentane radical cation, S. Lunell, L.A. Eriksson, T. Fängström, J. Maruani, L. Sjöqvist and A. Lund 171 (1993) 119
- An examination of the structure and inversion barrier for lithium and sodium phosphide, J.S. Francisco and G. Khitrov 171 (1993) 153
- Valence electron momentum distributions of the hydrogen halides. I. Comparison of EMS measurements and calculations using Hartree-Fock limit and configuration interaction wavefunctions for hydrogen fluoride, B.P. Hollebone, Y. Zheng, C.E. Brion, E.R. Davidson and D. Feller 171 (1993) 303
- The tetramer of borane and its heavier valence-isoelectronic analogs:  $M_4H_{12}$  with  $M=B$ , Al, and Ga, M. Shen, C. Liang and H.F. Schaefer III 171 (1993) 325
- $^1H$  and  $^2D$  electron nuclear double resonance (ENDOR) and electron spin echo envelope modulation (ESEEM) investigations on  $\gamma$ -irradiated betaine arsenate, A. Pöpl, G. Völkel, O. Tober, A. Klöpperpieper, J. Hüttermann and W. Gatzweiler 171 (1993) 375
- $^{14}N$  ENDOR study of  $\gamma$ -irradiated betaine arsenate, A. Pöpl and G. Völkel 171 (1993) 387

### *Vibrations and rotations of molecules*

- Analysis of the torsional Raman spectrum of a pyramidal molecule, dimethylamine, D. Consalvo, J.W.I. van Bladel, R. Engeln and J. Reuss 171 (1993) 221
- The tetramer of borane and its heavier valence-isoelectronic analogs:  $M_4H_{12}$  with  $M=B$ , Al, and Ga, M. Shen, C. Liang and H.F. Schaefer III 171 (1993) 325
- State-to-state cross sections for rotational excitation of ortho- and para- $NH_3$  by ortho- and para- $H_2$ . Experiment versus theory, J. Schleipen, J.J. ter Meulen and A.R. Offer 171 (1993) 347

### *Electronic structure and states*

- Cooperative core hole screening mechanism in adsorbates: its hindrance in the NEXAFS spectra of the CO/Ni and  $N_2$ /Ni systems, M. Ohno and P. Decleva 171 (1993) 9
- Quasidegenerate perturbation theory applied to the calculation of excitation spectra, A. Lisini, P. Decleva and G. Fronzoni 171 (1993) 159
- Ab initio calculations on the one- and two-photon electronic transitions of the conjugated isomers of benzene, V. Galasso 171 (1993) 171
- Optical excitation of the  $b^4\Sigma^- - X^2\Pi$  transition in NO, M.J. Dyer, G.W. Faris, P.C. Cosby, D.L. Huestis and T.G. Slanger 171 (1993) 237
- Stark effect and spectral hole-burning: solvation of organic dyes in polymers, E. Vauthey, K. Holliday, C. Wei, A. Renn and U.P. Wild 171 (1993) 253
- Energy gap equation of 1D polyconjugated  $\pi$ -systems in the Hubbard approximation, N. Tyutyulkov and F. Dietz 171 (1993) 293
- Ab initio CI calculation of nuclear quadrupole coupling constants of low-lying rovibrational levels in the  $X^1\Sigma^+$  state of  $CH^+$ , J. Fišer and J. Vojtk 171 (1993) 319

### *Electric and magnetic properties*

- Theoretical investigation of the structure and dynamics of the cyclopentane radical cation, S. Lunell, L.A. Eriksson, T. Fängström, J. Maruani, L. Sjöqvist and A. Lund 171 (1993) 119
- Hydration dependence of molecular mobility in phospholipid bilayers, P. Pissis, A. Enders and G. Nimtz 171 (1993) 285

*Molecular interactions*

- A new insight into the mechanism of intermolecular forces, E.A. Power and T. Thirunamachandran 171 (1993) 1
- State-to-state cross sections for rotational excitation of ortho- and para-NH<sub>3</sub> by ortho- and para-H<sub>2</sub>. Experiment versus theory, J. Schleipen, J.J. ter Meulen and A.R. Offer 171 (1993) 347

*Spectral bandshapes and intensities*

- Response functions and susceptibilities for multiresonant non-linear optical spectroscopy: perturbative computer algebra solution including feeding, B. Dick 171 (1993) 59
- Electro-absorption spectra of degenerate charge transfer states, P. Petelenz 171 (1993) 397

*Coupling of electronic and nuclear motion*

- Solvent effects on the torsional dynamics of a twisted intramolecular charge transfer (TICT) molecule: bianthryl in acetonitrile, M.J. Smith, K. Krogh-Jespersen and R.M. Levy 171 (1993) 97
- Coupled-wavepacket study of model dissociative charge exchange in collisions between a diatomic ion and a diatomic molecule, F. Aguilon, V. Sidis and J.P. Gauyacq 171 (1993) 363

*Energy transfer processes*

- Haken-Strobl-Reineker model: its limits of validity and a possible extension, V. Čápek 171 (1993) 79
- Tyrosine hypochromism and absence of tyrosine-tryptophan energy transfer in phospholipase A<sub>2</sub> and ribonuclease T<sub>1</sub>, N. Vekshin, M. Vincent and J. Gallay 171 (1993) 231
- Optical excitation of the b <sup>4</sup>Σ<sup>-</sup>-X <sup>2</sup>Π transition in NO, M.J. Dyer, G.W. Faris, P.C. Cosby, D.L. Fleet and T.G. Slanger 171 (1993) 237
- SO<sub>2</sub> fluorescence in cooled molecular beams under a magnetic field. The model analysis, K.A. Amosov, S.A. Kochubei, K.N. Naumochkin, V.I. Makarov, I.V. Khmelinski and N.M. Bazhin 171 (1993) 275
- State-to-state cross sections for rotational excitation of ortho- and para-NH<sub>3</sub> by ortho- and para-H<sub>2</sub>. Experiment versus theory, J. Schleipen, J.J. ter Meulen and A.R. Offer 171 (1993) 347

*Molecular photophysical processes*

- Orientation and alignment of <sup>2</sup>P<sub>3/2</sub> fragments following photodissociation of heteroatomic molecules, D.V. Kupriyanov and O.S. Vasyutinskii 171 (1993) 25
- Orientation and alignment of metastable <sup>2</sup>P<sub>3/2</sub> thallium atoms following photodissociation of TlBr, A.G. Evseev, D.V. Kupriyanov, B.V. Picheyev, B.N. Sevastianov and O.S. Vasyutinskii 171 (1993) 45
- Coherence effects in the anisotropy of optical experiments, K. Wynne and R.M. Hochstrasser 171 (1993) 179

*Intramolecular dynamics*

- Theoretical simulation of OH and OD stretching bands of isotopically diluted HDO molecules in aqueous solution, M.J. Wojcik, K. Hermansson, J. Lindgren and L. Ojamäe 171 (1993) 189

*-radiationless transitions*

- SO<sub>2</sub> fluorescence in cooled molecular beams under a magnetic field. The model analysis, K.A. Amosov, S.A. Kochubei, K.N. Naumochkin, V.I. Makarov, I.V. Khmelinski and N.M. Bazhin 171 (1993) 275

*Coherence loss processes*

- Coherence effects in the anisotropy of optical experiments, K. Wynne and R.M. Hochstrasser 171 (1993) 179



*Non-linear responses (including optical)*

- Response functions and susceptibilities for multiresonant non-linear optical spectroscopy: perturbative computer algebra solution including feeding, B. Dick 171 (1993) 59

*Multiphoton phenomena*

- Ab initio calculations on the one- and two-photon electronic transitions of the conjugated isomers of benzene, V. Galasso 171 (1993) 171

*Reactions (including dissociation)**-gas phase*

- A theoretical study of the collinear reaction  $F + H_2 \rightarrow HF + H$  using multiconfigurational second-order perturbation theory (CASPT2), R. González-Luque, M. Merchán and B.O. Roos 171 (1993) 107
- Kinetics of the reaction  $OH + NO + M \rightarrow HONO + M$  as a function of temperature and pressure in the presence of argon,  $SF_6$ , and  $N_2$  bath gas, S. Zabarnick 171 (1993) 265

*Electron transfer*

- Coupled-wavepacket study of model dissociative charge exchange in collisions between a diatomic ion and a diatomic molecule, F. Aguillon, V. Sidis and J.P. Gauyacq 171 (1993) 363

*Ionization (including Rydberg states)*

- Cooperative core hole screening mechanism in adsorbates: its hindrance in the NEXAFS spectra of the CO/Ni and  $N_2$ /Ni systems, M. Ohno and P. Decleva 171 (1993) 9

*Molecular motion (including diffusive)*

- Solvent effects on the torsional dynamics of a twisted intramolecular charge transfer (TICT) molecule: bianthryl in acetonitrile, M.J. Smith, K. Krogh-Jespersen and R.M. Levy 171 (1993) 97

*Isotopic effects*

- Isotope effects on the stability of the nitrogen-acetylene van der Waals dimer, S.A.C. McDowell and A.D. Buckingham 171 (1993) 89
- Vibrational study of various crystalline phases of thallium dihydrogen phosphate  $TiH_2PO_4$  and its deuterated analog  $TiD_2PO_4$ , B. Pasquier, N. Le Calvé, S. Al Homsí-Teiar and F. Fillaux 171 (1993) 203
- Ab initio CI calculation of nuclear quadrupole coupling constants of low-lying rovibrational levels in the  $X^1\Sigma^+$  state of  $CH^+$ , J. Fišer and J. Vojtík 171 (1993) 319

*Thermodynamic and transport properties*

- Hydration dependence of molecular mobility in phospholipid bilayers, P. Pissis, A. Enders and G. Nimtz 171 (1993) 285

*Phase transitions*

- Vibrational study of various crystalline phases of thallium dihydrogen phosphate  $TiH_2PO_4$  and its deuterated analog  $TiD_2PO_4$ , B. Pasquier, N. Le Calvé, S. Al Homsí-Teiar and F. Fillaux 171 (1993) 203



- <sup>1</sup>H and <sup>2</sup>D electron nuclear double resonance (ENDOR) and electron spin echo envelope modulation (ESEEM) investigations on  $\gamma$ -irradiated betaine arsenate, A. Pöpl, G. Völkel, O. Tober, A. Klöpperpieper, J. Hüttermann and W. Gatzweiler 171 (1993) 375
- <sup>14</sup>N ENDOR study of  $\gamma$ -irradiated betaine arsenate, A. Pöpl and G. Völkel 171 (1993) 387

